

10/524, 207

Connecting via Winsock to STN

1/4/06

Welcome to STN International! Enter x:x

LOGINID:SSSPTASXH1641

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America  
NEWS 2 "Ask CAS" for self-help around the clock  
NEWS 3 SEP 09 ACD predicted properties enhanced in REGISTRY/ZREGISTRY  
NEWS 4 OCT 03 MATHDI removed from STN  
NEWS 5 OCT 04 CA/CAPLUS-Canadian Intellectual Property Office (CIPO) added  
to core patent offices  
NEWS 6 OCT 13 New CAS Information Use Policies Effective October 17, 2005  
NEWS 7 OCT 17 STN(R) AnaVist(TM), Version 1.01, allows the export/download  
of CAPLUS documents for use in third-party analysis and  
visualization tools  
NEWS 8 OCT 27 Free KWIC format extended in full-text databases  
NEWS 9 OCT 27 DIOGENES content streamlined  
NEWS 10 OCT 27 EPFULL enhanced with additional content  
NEWS 11 NOV 14 CA/CAPLUS - Expanded coverage of German academic research  
NEWS 12 NOV 30 REGISTRY/ZREGISTRY on STN(R) enhanced with experimental  
spectral property data  
NEWS 13 DEC 05 CASREACT(R) - Over 10 million reactions available  
NEWS 14 DEC 14 2006 MeSH terms loaded in MEDLINE/LMEDLINE  
NEWS 15 DEC 14 2006 MeSH terms loaded for MEDLINE file segment of TOXCENTER  
NEWS 16 DEC 14 CA/CAPLUS to be enhanced with updated IPC codes  
NEWS 17 DEC 16 MARPATprev will be removed from STN on December 31, 2005  
NEWS 18 DEC 21 IPC search and display fields enhanced in CA/CAPLUS with the  
IPC reform  
NEWS 19 DEC 23 New IPC8 SEARCH, DISPLAY, and SELECT fields in USPATFULL/USPAT2  
  
NEWS EXPRESS JANUARY 03 CURRENT VERSION FOR WINDOWS IS V8.01,  
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),  
AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005.  
V8.0 USERS CAN OBTAIN THE UPGRADE TO V8.01 AT  
<http://download.cas.org/express/v8.0-Discover/>  
  
NEWS DCOST SINCE APPROXIMATELY 20:00 COLUMBUS TIME DECEMBER 29,  
SOME ONLINE COST DISPLAYS HAVE BEEN SHOWING COSTS IN  
2006 PRICES FOR STN COLUMBUS FILES. THIS HAS BEEN  
CORRECTED. PLEASE BE ASSURED THAT YOU WILL BE BILLED  
ACCORDING TO 2005 PRICES UNTIL JAN 1. PLEASE CONTACT  
YOUR LOCAL HELP DESK IF YOU HAVE ANY QUESTIONS. WE  
APOLOGIZE FOR THE ERROR.  
  
NEWS HOURS STN Operating Hours Plus Help Desk Availability  
NEWS INTER General Internet Information  
NEWS LOGIN Welcome Banner and News Items  
NEWS PHONE Direct Dial and Telecommunication Network Access to STN  
NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that  
specific topic.

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 16:56:19 ON 04 JAN 2006

=>

Uploading

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

Do you want to switch to the Registry File?

Choice (Y/n):

Switching to the Registry File...

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 16:56:31 ON 04 JAN 2006

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 3 JAN 2006 HIGHEST RN 871080-87-4

DICTIONARY FILE UPDATES: 3 JAN 2006 HIGHEST RN 871080-87-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

\*\*\*\*\*  
\*  
\* The CA roles and document type information have been removed from \*  
\* the IDE default display format and the ED field has been added, \*  
\* effective March 20, 2005. A new display format, IDERL, is now \*  
\* available and contains the CA role and document type information. \*  
\*  
\*\*\*\*\*

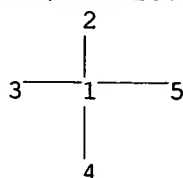
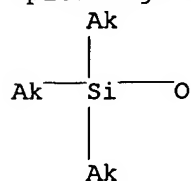
Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10524207.str



chain nodes :

1 2 3 4 5

chain bonds :

1-2 1-3 1-4 1-5

exact/norm bonds :

1-2 1-3 1-4

exact bonds :

1-5

Match level :

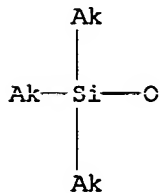
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 16:56:45 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 24460 TO ITERATE

8.2% PROCESSED 2000 ITERATIONS

50 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 479844 TO 498556

PROJECTED ANSWERS: 315021 TO 330233

L2 50 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 16:56:53 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 487896 TO ITERATE

100.0% PROCESSED 487896 ITERATIONS  
SEARCH TIME: 00.00.06

319576 ANSWERS

L3 319576 SEA SSS FUL L1

=> FIL CAPLUS

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

166.94

167.15

FILE 'CAPLUS' ENTERED AT 16:57:05 ON 04 JAN 2006

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE COVERS 1907 - 4 Jan 2006 VOL 144 ISS 2

FILE LAST UPDATED: 3 Jan 2006 (20060103/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s l3

TOO MANY TERMS FOR FILE CROSSOVER IN L3

There are limits on the size of an answer set being crossed over from one file to another. Enter HELP CROSSOVER at an arrow prompt (=>) for specific information.

=> help crossover

The term 'file crossover' refers to the use of an answer set L-number created by a search in one file as a search term or profile in another file. There are four types of crossovers in CAPLUS: query crossover, accession number crossover, crossover from the Registry File, and crossover of extracted terms.

The query is searched in CAPLUS when you search the L-number answer set created in another file, except for CASREACT, MARPAT, MARPATprev, and Registry.

Accession numbers are crossed over when you search an L-number answer set from CASREACT, MARPAT or MARPATprev in CAPLUS or when you search an L-number answer set from CAPLUS in MARPAT or MARPATprev.

You may use the CAS Registry Numbers(R) that are answers from a search in the REGISTRY File as a search term or profile in the CAPLUS File, without looking at all the answers or entering the Registry Numbers individually. To do this, enter the L-number of the REGISTRY answer set in a SEARCH command in CAPLUS. You may use this L-number

in any search where you might use a Registry Number, i.e., combined with other terms using the logical operators or the (L) operator. Registry Numbers crossed over from the REGISTRY File include all deleted (DR), replacing (RR), preferred (PR) and alternate (AR) numbers.

CAS Registry Numbers appended by D or DP are automatically searched whenever CAS Registry Numbers are crossed over. The suffix D indicates a generic or unspecified derivative, and DP indicates the preparation of generic derivatives. If you do not want to search CAS Registry Numbers for nonspecific derivatives, append the crossover L-number with /RN.

Examples (where L3 is an answer set from the REGISTRY File):

Search term	Retrieves
=> S L3	All CAS Registry numbers, including those appended with D or DP
=> S L3/RN	All CAS Registry Numbers, excluding those appended with D or DP

Additionally, the REGISTRY File answer set may be qualified by a code for a CAS Role. Enter HELP ROLES at an arrow prompt (=>) in this file to obtain a list of role codes and their definitions.

Example of a search for Registry Numbers with the role code ANT for the role of "analyte" (where L3 is an answer set from the REGISTRY File):

=> S L3/ANT

There is a limit of 300,000 answers for a single crossover of CAS Registry Numbers. For information on how to transfer more than 300,000 CAS Registry Numbers from the REGISTRY File, enter HELP CROSSOVER at an arrow prompt in REGISTRY.

You may also crossover and search a set of terms extracted from an answer set.

To crossover records from CAplus to CAOLD, use SELECT or TRANSFER with the OREF field. The OREF (Original Reference Number) field contains the Original Reference Number(s) for any record published in printed CA in 1907-1966. The format of OREF is the volume number of CA, colon, column number and fraction designation for the location of the entire bibliographic record and the abstract on the page of printed CA.

Enter HELP OREF for an example of a crossover from CAplus to CAOLD. For more information on crossover of extracted terms, enter HELP TRANSFER at an arrow prompt.

=> s l3/RN

TOO MANY TERMS FOR FILE CROSSOVER IN L3

There are limits on the size of an answer set being crossed over from one file to another. Enter HELP CROSSOVER at an arrow prompt (=>) for specific information.

=> s l3 and fluorine

TOO MANY TERMS FOR FILE CROSSOVER IN L3

There are limits on the size of an answer set being crossed over from

one file to another. Enter HELP CROSSOVER at an arrow prompt (=>) for specific information.

=> s l3/ant

TOO MANY TERMS FOR FILE CROSSOVER IN L3

There are limits on the size of an answer set being crossed over from one file to another. Enter HELP CROSSOVER at an arrow prompt (=>) for specific information.

=> s l3/fluorine

TOO MANY TERMS FOR FILE CROSSOVER IN L3

There are limits on the size of an answer set being crossed over from one file to another. Enter HELP CROSSOVER at an arrow prompt (=>) for specific information.

=> help crossover

The term 'file crossover' refers to the use of an answer set L-number created by a search in one file as a search term or profile in another file. There are four types of crossovers in CAlus: query crossover, accession number crossover, crossover from the Registry File, and crossover of extracted terms.

The query is searched in CAlus when you search the L-number answer set created in another file, except for CASREACT, MARPAT, MARPATprev, and Registry.

Accession numbers are crossed over when you search an L-number answer set from CASREACT, MARPAT or MARPATprev in CAlus or when you search an L-number answer set from CAlus in MARPAT or MARPATprev.

You may use the CAS Registry Numbers(R) that are answers from a search in the REGISTRY File as a search term or profile in the CAlus File, without looking at all the answers or entering the Registry Numbers individually. To do this, enter the L-number of the REGISTRY answer set in a SEARCH command in CAlus. You may use this L-number in any search where you might use a Registry Number, i.e., combined with other terms using the logical operators or the (L) operator. Registry Numbers crossed over from the REGISTRY File include all deleted (DR), replacing (RR), preferred (PR) and alternate (AR) numbers.

CAS Registry Numbers appended by D or DP are automatically searched whenever CAS Registry Numbers are crossed over. The suffix D indicates a generic or unspecified derivative, and DP indicates the preparation of generic derivatives. If you do not want to search CAS Registry Numbers for nonspecific derivatives, append the crossover L-number with /RN.

Examples (where L3 is an answer set from the REGISTRY File):

Search term	Retrieves
=> S L3	All CAS Registry numbers, including those appended with D or DP
=> S L3/RN	All CAS Registry Numbers, excluding those appended with D or DP

Additionally, the REGISTRY File answer set may be qualified by a code for a CAS Role. Enter HELP ROLES at an arrow prompt (=>) in this file to obtain a list of role codes and their definitions.

Example of a search for Registry Numbers with the role code ANT for the role of "analyte" (where L3 is an answer set from the REGISTRY File):

=> S L3/ANT

There is a limit of 300,000 answers for a single crossover of CAS Registry Numbers. For information on how to transfer more than 300,000 CAS Registry Numbers from the REGISTRY File, enter HELP CROSSOVER at an arrow prompt in REGISTRY.

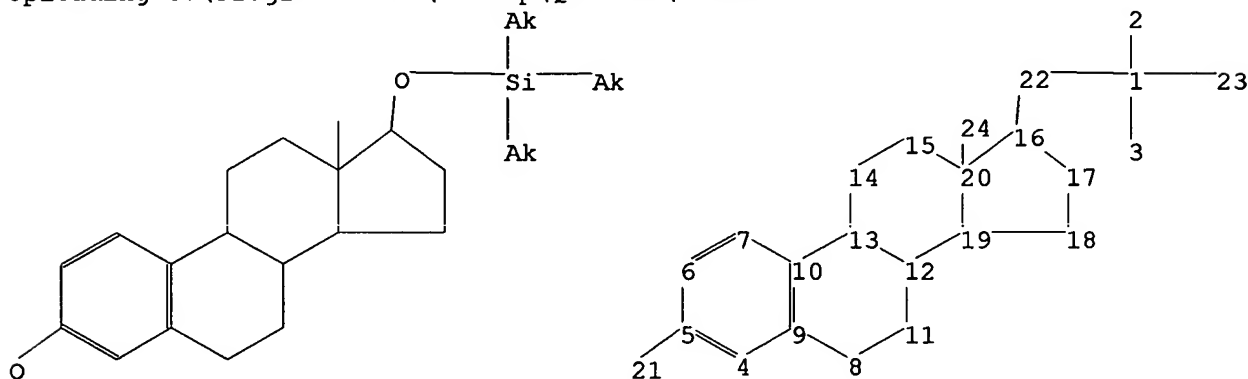
You may also crossover and search a set of terms extracted from an answer set.

To crossover records from CAPLUS to CAOLD, use SELECT or TRANSFER with the OREF field. The OREF (Original Reference Number) field contains the Original Reference Number(s) for any record published in printed CA in 1907-1966. The format of OREF is the volume number of CA, colon, column number and fraction designation for the location of the entire bibliographic record and the abstract on the page of printed CA.

Enter HELP OREF for an example of a crossover from CAplus to CAOLD.  
For more information on crossover of extracted terms, enter HELP  
TRANSFER at an arrow prompt.

 $\Rightarrow$ 

Uploading C:\Program Files\Stnexp\Queries\10524207a.str



```
chain nodes :
```

1    2    3    21    22    23    24

```
ring nodes :
```

4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

chain bonds :

1-2   1-3   1-22   1-23   5-21   16-22   20-24

ring bonds :

4-5 4-9 5-6 6-7 7-10 8-9 8-11 9-10 10-13 11-12 12-13 12-19 13-14 14-15  
15-20 16-17 16-20 17-18 18-19 19-20

exact/norm bonds :

1-2    1-3    1-23    5-21    16-22

exact bonds :

1-22	8-9	8-11	10-13	11-12	12-13	12-19	13-14	14-15	15-20	16-17	16-20
17-18	18-19	19-20	20-24								

normalized bonds :

4-5    4-9    5-6    6-7    7-10    9-10

isolated ring systems :

containing 4 :

Match level :

1:CLASS 2:CLASS 3:CLASS 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom  
20:Atom 21:CLASS 22:CLASS 23:CLASS 24:CLASS

L4 STRUCTURE UPLOADED

=> FIL REGISTRY

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

9.66

176.81

FILE 'REGISTRY' ENTERED AT 17:09:25 ON 04 JAN 2006  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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STRUCTURE FILE UPDATES: 3 JAN 2006 HIGHEST RN 871080-87-4

DICTIONARY FILE UPDATES: 3 JAN 2006 HIGHEST RN 871080-87-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

\*\*\*\*\*  
\*  
\* The CA roles and document type information have been removed from \*  
\* the IDE default display format and the ED field has been added, \*  
\* effective March 20, 2005. A new display format, IDERL, is now \*  
\* available and contains the CA role and document type information. \*  
\*  
\*\*\*\*\*

Structure search iteration limits have been increased. See HELP SLIMITS  
for details.

REGISTRY includes numerically searchable data for experimental and  
predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=> s 14

SAMPLE SEARCH INITIATED 17:09:31 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 67 TO ITERATE

100.0% PROCESSED

67 ITERATIONS

22 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 849 TO 1831  
PROJECTED ANSWERS: 159 TO 721

L5 22 SEA SSS SAM L4

=> s 15 sss full  
FULL SEARCH INITIATED 17:09:45 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 1390 TO ITERATE

100.0% PROCESSED 1390 ITERATIONS 518 ANSWERS  
SEARCH TIME: 00.00.01

L6 518 SEA SSS FUL L4

=> FIL CAPLUS  
COST IN U.S. DOLLARS SINCE FILE TOTAL  
ENTRY SESSION  
FULL ESTIMATED COST 166.94 343.75

FILE 'CAPLUS' ENTERED AT 17:09:50 ON 04 JAN 2006  
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FILE COVERS 1907 - 4 Jan 2006 VOL 144 ISS 2  
FILE LAST UPDATED: 3 Jan 2006 (20060103/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s 16  
L7 165 L6

=> s 17 and (fluoride or fluorine)  
244734 FLUORIDE  
44140 FLUORIDES  
260172 FLUORIDE  
(FLUORIDE OR FLUORIDES)  
98401 FLUORINE  
521 FLUORINES  
98691 FLUORINE  
(FLUORINE OR FLUORINES)  
L8 4 L7 AND (FLUORIDE OR FLUORINE)

=> d l8 ibib abs hitstr tot

L8 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 2004:1037341 CAPLUS  
DOCUMENT NUMBER: 142:18635  
TITLE: Determination of **fluoride** or hydrogen

**fluoride** in environmental samples  
 INVENTOR(S): Ezan, Eric; Sagot, Marie-Astrid; Pradelles, Philippe  
 PATENT ASSIGNEE(S): Commissariat a l'Energie Atomique, Fr.  
 SOURCE: PCT Int. Appl., 83 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: French  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004104579	A1	20041202	WO 2004-FR50194	20040514
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
FR 2865540	A1	20050729	FR 2003-50160	20030520
FR 2865541	A1	20050729	FR 2003-50167	20030522
CA 2495558	AA	20041202	CA 2004-2495558	20040514
BR 2004006175	A	20050719	BR 2004-6175	20040514
US 2005227368	A1	20051013	US 2005-524207	20050210
PRIORITY APPLN. INFO.:			FR 2003-50160	A 20030520
			FR 2003-50167	A 20030522
			WO 2004-FR50194	W 20040514

OTHER SOURCE(S): MARPAT 142:18635

AB The invention relates to a method for the detection and/or determination of **fluoride** or HF in a sample. The sample is treated with a silylated organic compound in an aqueous solution in order to obtain a measuring solution. The organic silyl compound is desilylated by **fluoride** or HF, whereby the silylated organic compound and the desilylated organic compound can be detected and/or dosed in a distinct manner. The appearance of the desilylated organic compound or the disappearance of the organic silylated compound which occurs if **fluoride** or hydrogen **fluoride** is present, is determined in the measuring solution. The silylated organic compounds are estradiol, peptides, homovanillic acid, amphotericin, steroids, cytokines and arachidonic acid. The silylated organic compounds and the desilylated organic compound can be detected and determined by gas chromatog. or immunoassay. The invention makes it possible to detect in a very practical and easy manner the presence of HF or **fluoride** in concns. of 10<sup>-2</sup> L of/ 10<sup>6</sup> L air (10 ppb), or even 0.5-1 g/mL HF in a solution. The inventive kit comprises the elements which are required to carry out said method. The inventive method makes it possible to detect **fluoride** in concns. of 0,001 g/mL.

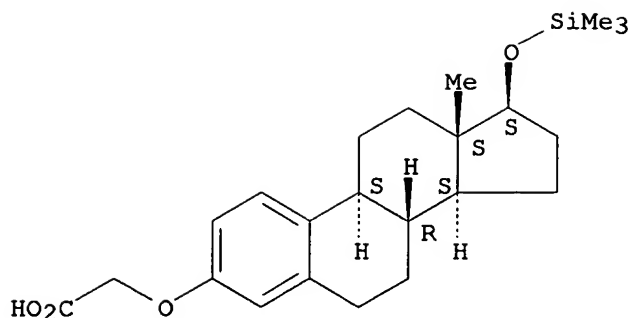
IT 799775-62-5

RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
 (reagent in determination of **fluoride** or hydrogen **fluoride** in environmental samples)

RN 799775-62-5 CAPLUS

CN Acetic acid, [[(17 $\beta$ )-17-[(trimethylsilyl)oxy]estra-1,3,5(10)-trien-3-yl]oxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:465104 CAPLUS

DOCUMENT NUMBER: 141:153363

TITLE: Detection of chemicals by a reporter immunoassay: Application to **fluoride**

AUTHOR(S): Sagot, Marie-Astrid; Heutte, Florence; Renard, Pierre-Yves; Dolle, Frederic; Pradelles, Philippe; Ezan, Eric

CORPORATE SOURCE: Service de Pharmacologie et d'Immunologie, CEA, Mont St-Aignan, 76131, Fr.

SOURCE: Analytical Chemistry (2004), 76(15), 4286-4291  
CODEN: ANCHAM; ISSN: 0003-2700

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB This report describes a concept in which an immunoassay is used indirectly to quantify a nonantigenic very low mol. weight compound participating in a chemical reaction with a haptenic reporter. The detection limit of each reagent is, therefore, governed only by the affinity of the antibodies toward the reporter. **Fluoride** was used as a model, and silylated estradiol was used as a reporter. Upon silylation with N-O-bis(trimethylsilyl)trifluoroacetamide (BSTFA) or N-O-bis(dimethylterbutylsilyl) trifluoroacetamide (MTBSTFA), estradiol is no longer recognized by antibodies specific to estradiol. After reaction with hydrofluoric acid (HF) or **fluoride** salts (KF, CsF, NaF), its immunoreactivity is restored, and native estradiol is formed and is detected by immunoassay. The level of synthesized estradiol is dependent on the concentration of **fluoride**. A **fluoride** detection limit of 0.3 µg/L (15 nM) is obtained. Potential interference with other acids has been eliminated by choosing the silyl group (trimethylsilyl vs. tert-butyldimethylsilyl) and by selecting optimal reaction conditions for the desilylation. The method has been applied to the detection of **fluoride** salts in natural waters (range 0.28-9.0 mg/L) and in an atmospheric artificially contaminated with HF between 8 and 160 µg/m<sup>3</sup> in the parts-per-billion range. This indirect immunoassay combines simplicity and high sensitivity and, therefore, can be used in field monitoring. Finally, the extension of the concept to other chems. is discussed.

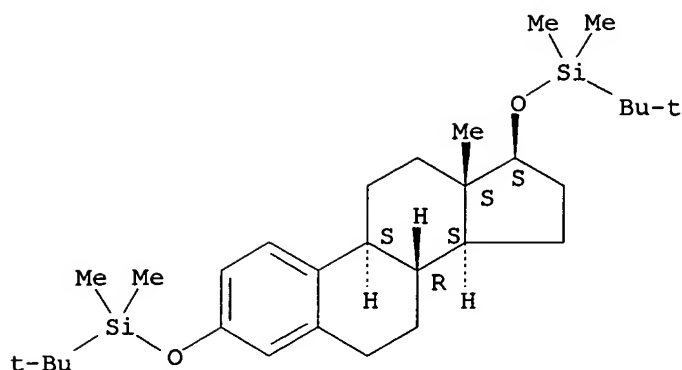
IT 57711-41-8P 96013-91-1P

RL: ARU (Analytical role, unclassified); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation)  
(detection of chems. by reporter immunoassay)

RN 57711-41-8 CAPLUS

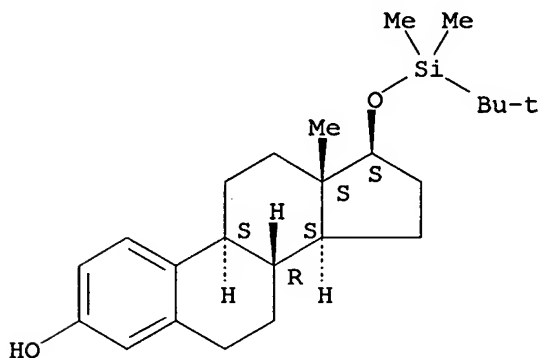
CN Silane, [[(17β)-estra-1,3,5(10)-triene-3,17-diyl]bis(oxy)]bis[(1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 96013-91-1 CAPLUS  
 CN Estra-1,3,5(10)-trien-3-ol, 17-[[ (1,1-dimethylethyl)dimethylsilyl]oxy]-,  
 (17 $\beta$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:751091 CAPLUS

DOCUMENT NUMBER: 124:30103

TITLE: A Novel 1,3 O  $\rightarrow$  C Silyl Shift and Deacylation  
 Reaction Mediated by Tetra-n-butylammonium  
**Fluoride** in an Aromatic System

AUTHOR(S): He, Hu-Ming; Fanwick, Phillip E.; Wood, Karl; Cushman,  
 Mark

CORPORATE SOURCE: Department of Medicinal Chemistry and Pharmacognosy,  
 Purdue University, West Lafayette, IN, 47907, USA

SOURCE: Journal of Organic Chemistry (1995), 60(18), 5905-9  
 CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 124:30103

AB A novel 1,3 O  $\rightarrow$  C migration of a silyl group accompanied by a  
 deacylation reaction was discovered during the conversion of  
 2-acetyl-3,17-bis(tert-butyldimethylsilyl)- $\beta$ -estradiol and  
 3,17-bis(tert-butyldimethylsilyl)-2-propionyl- $\beta$ -estradiol to  
 2,17-bis(tert-butyldimethylsilyl)- $\beta$ -estradiol in the presence of  
 tetra-n-butylammonium **fluoride**. A crossover experiment indicated  
 that the transformation is intramol.

IT 168131-85-9P 168131-86-0P 168131-87-1P  
168131-88-2P 168131-89-3P 168131-92-8P  
168131-93-9P

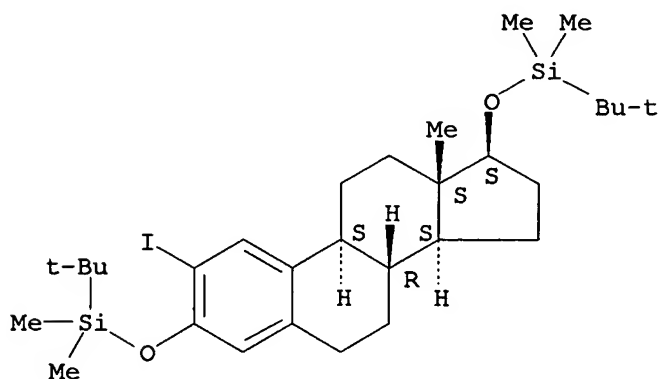
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

(a novel silyl shift and deacylation reaction mediated by  
tetra-n-butylammonium **fluoride** in aromatic system)

RN 168131-85-9 CAPLUS

CN Silane, [[(17 $\beta$ )-2-iodoestra-1,3,5(10)-triene-3,17-  
diyl]bis(oxy)]bis[(1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)

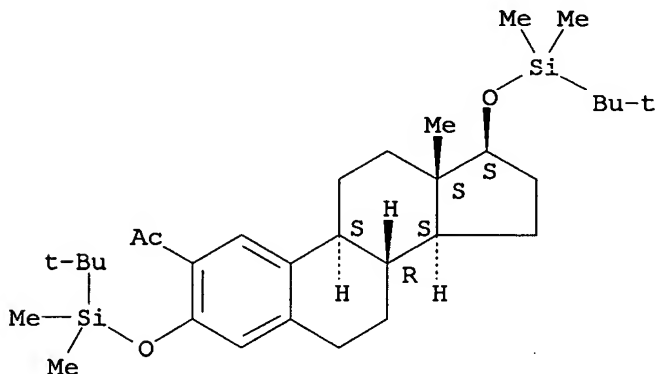
Absolute stereochemistry.



RN 168131-86-0 CAPLUS

CN Ethanone, 1-[(17 $\beta$ )-3,17-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]ester]-1,3,5(10)-trien-2-yl]- (9CI) (CA INDEX NAME)

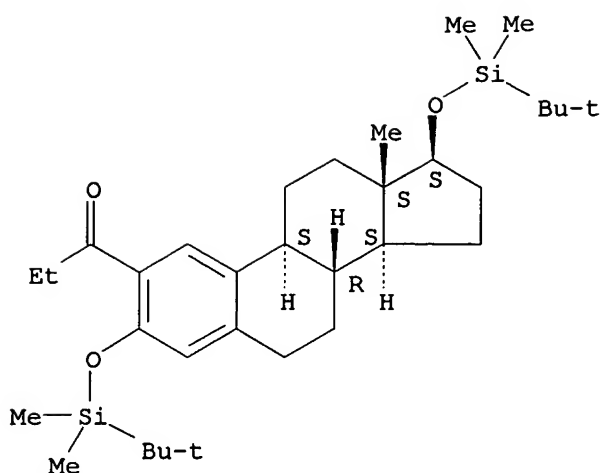
Absolute stereochemistry.



RN 168131-87-1 CAPLUS

CN 1-Propanone, 1-[(17 $\beta$ )-3,17-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]ester]-1,3,5(10)-trien-2-yl]- (9CI) (CA INDEX NAME)

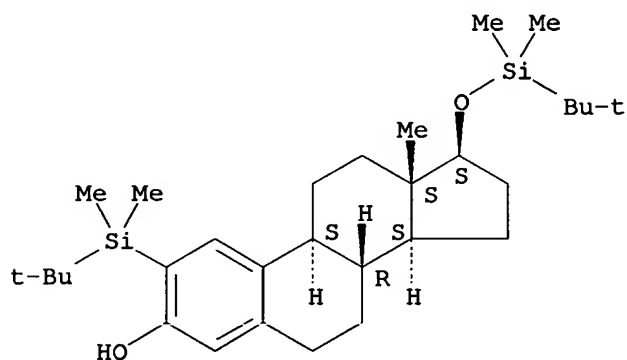
Absolute stereochemistry.



RN 168131-88-2 CAPLUS

CN Estradiol 17-((1,1-dimethylethyl)dimethylsilyl) ether 3-O-((1,1-dimethylethyl)dimethylsilyl) ether, (17 $\beta$ )- (9CI) (CA INDEX NAME)

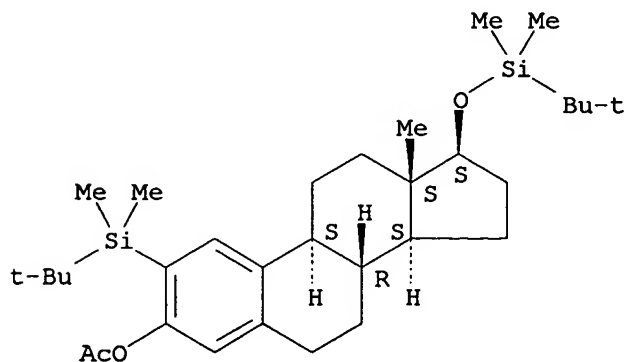
Absolute stereochemistry.



RN 168131-89-3 CAPLUS

CN Estradiol 17-((1,1-dimethylethyl)dimethylsilyl) ether 3-OH, acetate, (17 $\beta$ )- (9CI) (CA INDEX NAME)

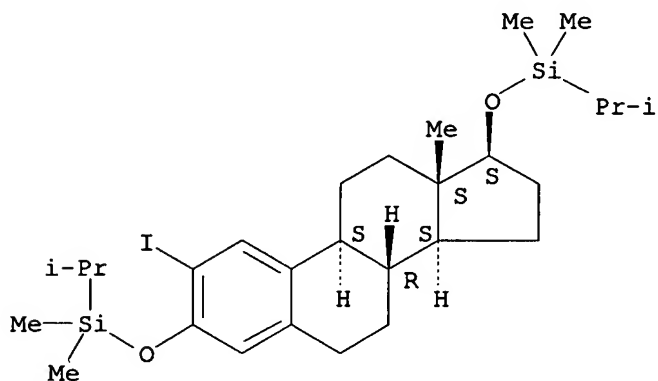
Absolute stereochemistry.



RN 168131-92-8 CAPLUS

CN Silane, [[(17 $\beta$ )-2-iodoestra-1,3,5(10)-triene-3,17-diyl]bis(oxy)]bis[dimethyl(1-methylethyl)- (9CI) (CA INDEX NAME)

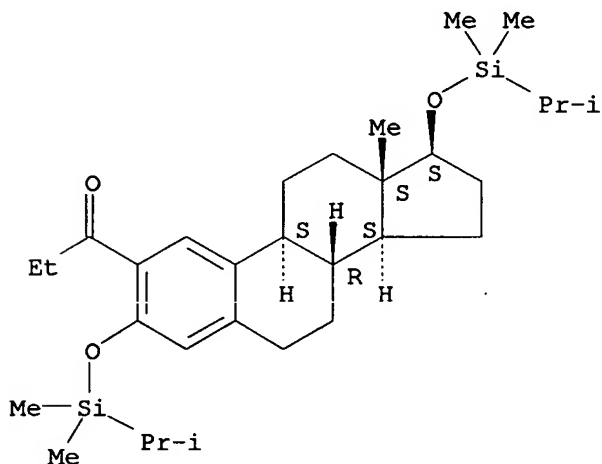
Absolute stereochemistry.



RN 168131-93-9 CAPLUS

CN 1-Propanone, 1-[(17 $\beta$ )-3,17-bis[[dimethyl(1-methylethyl)silyl]oxy]estra-1,3,5(10)-trien-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



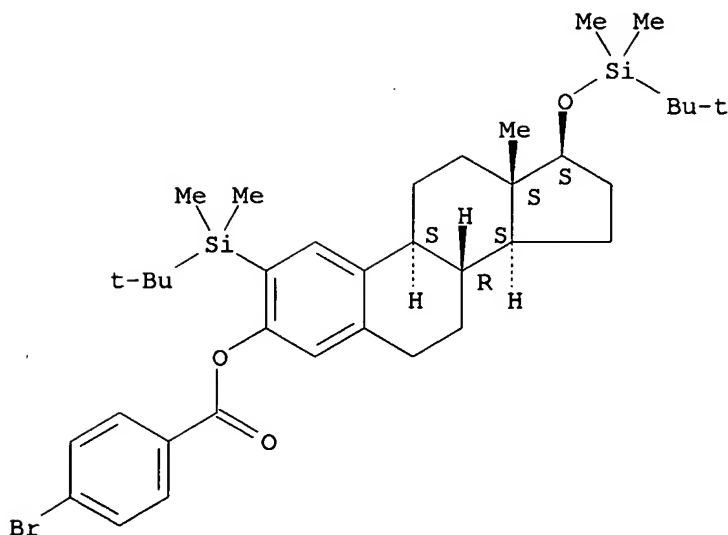
IT 168131-90-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(a novel silyl shift and deacylation reaction mediated by tetra-n-butylammonium **fluoride** in aromatic system)

RN 168131-90-6 CAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 2-[(1,1-dimethylethyl)dimethylsilyl]-17-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-, 4-bromobenzoate, (17 $\beta$ )- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1985:165979 CAPLUS

DOCUMENT NUMBER: 102:165979

TITLE: Selective deprotection of alcoholic and phenolic silyl ethers

AUTHOR(S): Collington, Eric W.; Finch, Harry; Smith, Ian J.

CORPORATE SOURCE: Chem. Res. Dep., Glaxo Group Res. Ltd.,  
Ware/Hertfordshire, SG12 0DJ, UK

SOURCE: Tetrahedron Letters (1985), 26(5), 681-4

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 102:165979

AB The selective deprotection of alc. or phenolic tert-butyldimethylsilyl ethers is described. The alc. ethers are deprotected with aqueous HF in MeCN, whereas phenolic ethers are deprotected with Bu<sub>4</sub>N<sup>+</sup>F<sup>-</sup> in THF.

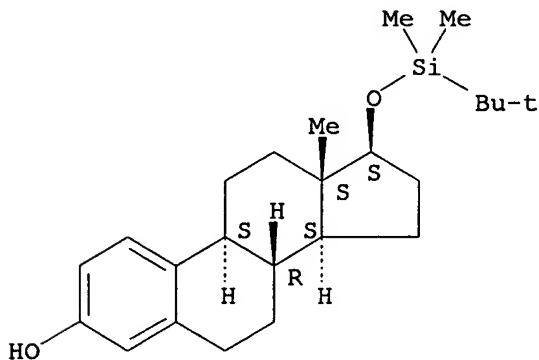
IT **96013-91-1P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 96013-91-1 CAPLUS

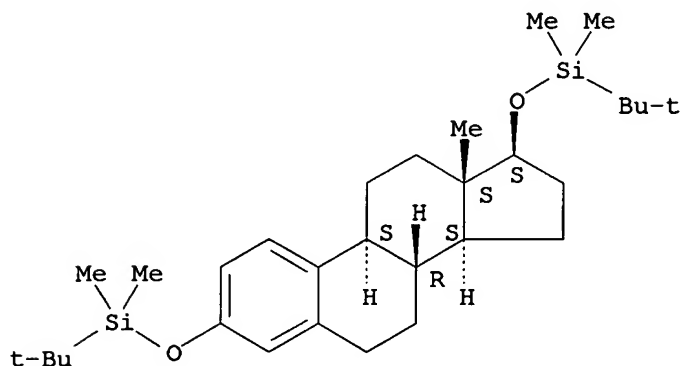
CN Estradiol, 17-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-,  
(17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 57711-41-8  
 RL: PROC (Process)  
 (selective deprotection of, with hydrogen fluoride or  
 tetrabutylammonium fluoride)  
 RN 57711-41-8 CAPLUS  
 CN Silane, [[(17 $\beta$ )-estra-1,3,5(10)-triene-3,17-diyl]bis(oxy)]bis[(1,1-  
 dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> FIL REGISTRY		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	28.02	371.77
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-3.00	-3.00

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\*\*\*\*\*  
 \*  
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 \* the IDE default display format and the ED field has been added, \*  
 \* effective March 20, 2005. A new display format, IDERL, is now \*  
 \* available and contains the CA role and document type information. \*  
 \*  
 \*\*\*\*\*

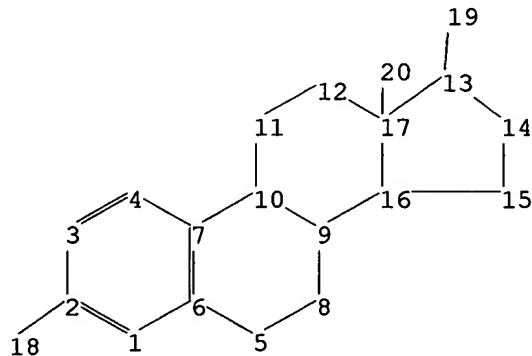
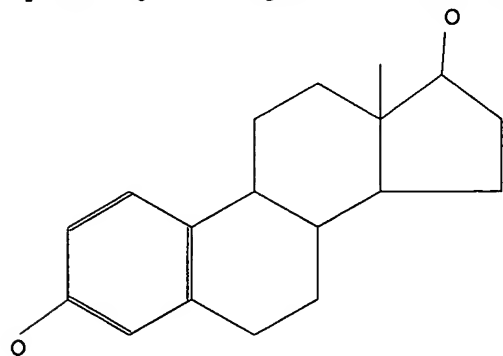
Structure search iteration limits have been increased. See HELP SLIMITS for details.

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<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10524207b.str



chain nodes :

18 19 20

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17

chain bonds :

2-18 13-19 17-20

ring bonds :

1-2 1-6 2-3 3-4 4-7 5-6 5-8 6-7 7-10 8-9 9-10 9-16 10-11 11-12 12-17  
13-14 13-17 14-15 15-16 16-17

exact/norm bonds :

2-18 13-19

exact bonds :

5-6 5-8 7-10 8-9 9-10 9-16 10-11 11-12 12-17 13-14 13-17 14-15 15-16  
16-17 17-20

normalized bonds :

1-2 1-6 2-3 3-4 4-7 6-7

isolated ring systems :

containing 1 :

Match level :

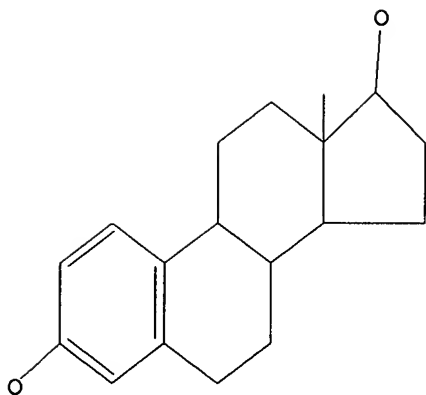
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS  
20:CLASS

L9 STRUCTURE UPLOADED

=> d 19

L9 HAS NO ANSWERS

L9 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 19

SAMPLE SEARCH INITIATED 17:15:17 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 1646 TO ITERATE

100.0% PROCESSED 1646 ITERATIONS 50 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 30487 TO 35353  
PROJECTED ANSWERS: 13017 TO 16263

L10 50 SEA SSS SAM L9

=> s 19 sss full

FULL SEARCH INITIATED 17:15:25 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 32777 TO ITERATE

100.0% PROCESSED 32777 ITERATIONS 14455 ANSWERS  
SEARCH TIME: 00.00.01

L11 14455 SEA SSS FUL L9

=> FIL CAPLUS

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	166.94	538.71
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-3.00

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FILE LAST UPDATED: 3 Jan 2006 (20060103/ED)

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<http://www.cas.org/infopolicy.html>

=> s l11

L12 75208 L11

=> s l12 and (fluoride or fluorine)

244734 FLUORIDE

44140 FLUORIDES

260172 FLUORIDE

(FLUORIDE OR FLUORIDES)

98401 FLUORINE

521 FLUORINES

98691 FLUORINE

(FLUORINE OR FLUORINES)

L13 232 L12 AND (FLUORIDE OR FLUORINE)

=> s l13 and (detect? or measur?)

1528769 DETECT?

2816615 MEASUR?

L14 45 L13 AND (DETECT? OR MEASUR?)

=> s l14 and (silicon or silica or silylat?)

750020 SILICON

445 SILICONS

750180 SILICON

(SILICON OR SILICONS)

487203 SILICA

3723 SILICAS

487613 SILICA

(SILICA OR SILICAS)

25297 SILYLAT?

L15 3 L14 AND (SILICON OR SILICA OR SILYLAT?)

=> s l15 not l8

L16 1 L15 NOT L8

=> d l16 ibib abs hitstr tot

L16 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1983:83043 CAPLUS

DOCUMENT NUMBER: 98:83043

TITLE: Boron trifluoride etherate as a spray reagent for the  
**detection** of steroids and triterpenoids by TLC  
AUTHOR(S): Ghosh, Parthasarathi; Thakur, Swapnadip  
CORPORATE SOURCE: Dep. Chem., Univ. Burdwan, Burdwan, 713104, India  
SOURCE: Fresenius' Zeitschrift fuer Analytische Chemie (1982),  
313(2), 144

CODEN: ZACFAU; ISSN: 0016-1152

DOCUMENT TYPE: Journal

LANGUAGE: English

AB B trifluoride etherate was used as a spray reagent for the **detection** of steroids and triterpenoids on **silica** gel-G thin-layer chromatog. (TLC) plates. After developing with 1:1 benzene-EtOAc, the plates were sprayed with the reagent and heated for 5 min at 125° to produce colored spots. The color reactions and **detection** limits are given for some steroids and triterpenoids.

IT 50-28-2, analysis 57-63-6 72-33-3

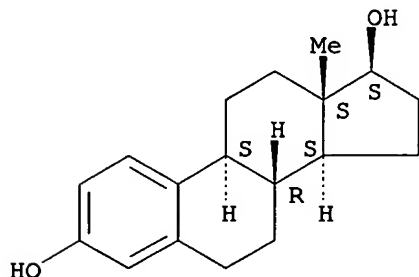
RL: ANT (Analyte); ANST (Analytical study)

(**detection** of, boron trifluoride etherate in thin-layer chromatog.)

RN 50-28-2 CAPLUS

CN Estra-1,3,5(10)-triene-3,17-diol (17β)- (9CI) (CA INDEX NAME)

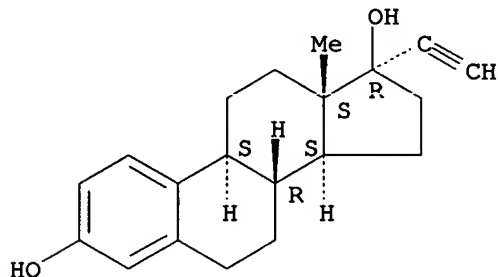
Absolute stereochemistry.



RN 57-63-6 CAPLUS

CN 19-Norpregna-1,3,5(10)-trien-20-yne-3,17-diol, (17α)- (9CI) (CA INDEX NAME)

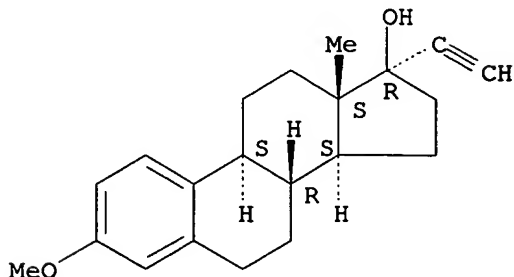
Absolute stereochemistry.



RN 72-33-3 CAPLUS

CN 19-Norpregna-1,3,5(10)-trien-20-yn-17-ol, 3-methoxy-, (17α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



```

=> s l14 and hydrofluoric acid
    23005 HYDROFLUORIC
    4081719 ACID
    1505424 ACIDS
    4567282 ACID
        (ACID OR ACIDS)
    22560 HYDROFLUORIC ACID
        (HYDROFLUORIC(W)ACID)
L17          1 L14 AND HYDROFLUORIC ACID

```

```

=> s l17 not l8
L18          0 L17 NOT L8

```

```

=> s l14 and fluorine
    98401 FLUORINE
    521 FLUORINES
    98691 FLUORINE
        (FLUORINE OR FLUORINES)
L19          22 L14 AND FLUORINE

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=> s l19 and silyla?
    29955 SILYLA?
L20          0 L19 AND SILYLA?

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=> log y		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	33.46	572.17
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
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CA SUBSCRIBER PRICE	-0.75	-3.75

STN INTERNATIONAL LOGOFF AT 17:24:16 ON 04 JAN 2006